Kinetic energy driven superconductivity
and pseugogap phase in weakly doped antiferromagnets

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We derive an effective Hamiltonian for spin polarons forming in weakly doped antiferromagnets and demonstrate that the system becomes superconducting at finite doping. We argue that the driving mechanism which gives rise to superconductivity is lowering of the kinetic energy by formation of mobile antiferromagnetic spin bipolarons. That source of attraction between holes is by definition effective if the antiferromagnetic correlation length is longer than the radius of forming polarons. Notwithstanding that the attraction is strongest in the undoped system with long range order, the superconducting order parameter vanishes when the doping parameter decreases which should be attributed to emptying the spin polaron band and approaching the Mott insulator phase. Since the hypothetical normal phase of low density gas of fermions is unstable against formation of bound hole pairs the intensity of low energy excitations is suppressed and the pseudogap forms in the underdoped region.

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I. INTRODUCTION

The appearance of superconductivity (SC) with high T_c in doped antiferromagnetic (AF) insulators belongs to most intriguing problems with which the contemporary condensed matter physics is confronted. A common feature of the family of systems which reveals that phenomenon is the presence of a building block in the form of copper-oxygen planes. On the other hand, this class of materials contains many compounds, properties of which are different in respect of many details. Thus a task of formulating a universal model capable of describing simultaneously all experimental aspects of cuprates seems elusive. Nevertheless some general understanding of SC in doped AF may be gained from analysis of a minimal model for such systems which is the t-J model (TJM).

Only recent numerical calculations based on combination of various techniques, like quantum Monte Carlo (QMC) and Lanczos algorithms, performed for relatively large clusters provided convincing evidence for pairing in the TJM[1,2]. These calculations also indicate that short-range AF correlations are robust even for moderate doping. Some time ago an effective model was suggested to discuss SC in the TJM[3]. According to that suggestion the driving attractive force between holes may be attributed to the fact that by sharing a common link two holes minimize the the loss of the energy related to breaking AF links. This effect was represented in that effective model by a term corresponding to attraction between holes created at nearest neighbor sites. According to a different point of view, pairing in doped AF is mediated by the exchange of spin waves[4,5]. In this paper we shall demonstrate that the main energetic gain in the paired state is due to formation of spin bipolarons which move in a way that saves the kinetic energy.

Detailed knowledge about binding in weakly doped AF, about the role which symmetry plays in this process[6] and about the internal structure of the bound pair indicates that the static attraction between holes related to minimization of the number of broken AF bonds if a hole pair occupies nearest neighbor sites is ineffective because in the interesting parameter region $t \gg J$ the kinetic energy of each hole is raised due to the presence of the second hole at a nearest neighbor site, which restricts the freedom of hole motion. That insight gained by means of the spin polaron (string) approach based on an assumption that short-range AF correlations prevail even for moderate doping has been verified by extensive comparisons with results of numerical analyses including QMC[7], exact diagonalization (ED)[8,9] and density matrix renormalization group (DMRG) calculations[10]. A consistent picture which emerges from the collection of different pieces of data is that competition between different phases like the non-superconducting local pair phase, the SC state, phase separation, or the stripe phase is governed by an obvious tendency to lower simultaneously the kinetic and the magnetic exchange energy. That conclusion is only seemingly trivial, because not like for a weakly correlated system, in which case the balance between the kinetic and the potential energy takes more conventional forms, the system has to resort to some tricky ways to achieve that goal, for example by forming anti-phase AF domains in the stripe phase[11].

In this paper, using knowledge gained about binding of holes in weakly doped AF[6], we analyze formation of the SC state in such a system in terms of an effective model, which represents propagation and interaction of spin polarons. The basic assumption of this approach is

that the AF correlation length is longer than the radius of spin polarons which seems to be valid at least in the region of weak doping. We will demonstrate that the shape of the curve representing the superconducting order parameter as a function of doping obtained in the numerical calculations[1] is reproduced within the Hartree Fock (HF) approximation to an effective Hamiltonian represented in the basis of spin polaron states and that the agreement for underdoped systems where the spin polaron approach should be valid is satisfactory.

The standard version of the TJM[12] on the square lattice is used in this article,

$$H = -t \sum_{\langle i,j \rangle, \sigma} \left(\hat{c}_{i,\sigma}^\dagger \hat{c}_{j,\sigma} + H.c. \right) + J \sum_{\langle i,j \rangle} \left(\mathbf{S}_i \mathbf{S}_j - \frac{n_i n_j}{4} \right). \tag{1}$$

The $\mathbf{S_i}$ are electronic spin operators, $\hat{c}_{i,\sigma}^\dagger = c_{i,\sigma}^\dagger \left(1 - n_{i,-\sigma} \right)$ and the sum over $\langle i, j \rangle$ stands for a summation over all pairs of nearest neighbors.

II. LOCALIZED SPIN POLARONS AND BIPOLARONS

The spin polaron approach[13–15] to binding of holes in doped AF is based on the notion of a string. A moving hole inserted into AF medium creates a line of defects (string) in the spin pattern, which raises the magnetic, potential-like contribution to the energy. Since the rate of processes related to hopping is higher than the rate of magnetic exchange processes during which anti-parallel spins on nearest neighbor sites are turned upside down, the latter category of processes may be temporarily neglected in the lowest order approximation, when a trial 'unperturbed' Hamiltonian H_0 is solved. That Hamiltonian represents a hole attached to a site by a string, or in other words it describes a particle in a potential well. The eigenstates of the trial Hamiltonian which we call in our terminology spin polarons span in principle the whole Hilbert space, but to discuss the low energy properties of the system it is sufficient to concentrate on the ground-state, which may be represented as,

$$|\Psi_i\rangle = \sum_{\mathcal{P}_i} \alpha_{l(\mathcal{P}_i)} |\mathcal{P}_i\rangle. \tag{2}$$

$|\mathcal{P}_i\rangle$ denotes a state obtained by hopping along a path $\mathcal{P}_i$ without retreats of a hole created at the site i in the AF medium. For simplicity, we assume that the Néel state plays the role of that medium and that amplitudes $\alpha_{l(\mathcal{P}_i)}$ depend only on the length of paths $l(\mathcal{P}_i)$. If more holes are created at distant sites, the wave function of multi-hole spin polaron representing many holes in separate potential wells is just a product of wave functions for single independent polarons. If a hole pair is created at nearest neighbor sites that approximation can not be applied, because the holes share the same region in which the spin arrangement has been disturbed. Due to the size reduction of the disturbed area, the increase of the static potential contribution to the energy related the part of the Hamiltonian which is equivalent to the Ising model, is reduced. On the other hand, proximity of holes may restrict their freedom of motion which raises the kinetic energy. In order to analyze quantitatively these effects we define a localized spin bipolaron as a combination of states which may be obtained by non-retraceable hopping of holes created at a pair of nearest neighbor sites i, j,

$$|\Psi_{i,j}\rangle = \sum_{\mathcal{P}_i, \mathcal{P}_j} \alpha_{l(\mathcal{P}_i), l(\mathcal{P}_j)} |\mathcal{P}_i, \mathcal{P}_j\rangle. \tag{3}$$

The amplitudes $\alpha_{l(\mathcal{P}_i), l(\mathcal{P}_j)}$ represent the groundstate solution of an approximate Schrödinger equation which describes two particles in the same potential well. More details concerning the construction of spin polarons may be found in earlier papers devoted to analysis of hole binding[13,14,6]. A general lesson which we learn by comparing eigenenergies of localized single polarons and bipolarons is that the gain in the energy related to the reduction of the number of broken bonds when holes occupy nearest neighbor sites is compensated by the loss of the kinetic energy which may be attributed to the fact that motion of each hole toward its partner is prohibited in such a case.

III. EFFECTIVE HAMILTONIAN

During the process of construction of spin polarons we have solved a trial 'unperturbed' Hamiltonian which is a part of the full TJM. We will take into account the remaining part of the TJM by analyzing all processes which have been neglected at the earlier stage of the calculation. We will express these processes in terms of a Hamiltonian matrix which couples spin polaron states. This way of expressing the TJM is very convenient, because eigenenergies of a spin polaron and a spin bipolaron already contain a substantial part of the energy related to the fast incoherent motion of holes inside potential wells. The formulation of the Hamiltonian in terms of the spin-polaron basis brings about some new features of the formalism. Since spin bipolaron states are not orthogonal, the particle-number operator contains two-body terms which consist of a pair of operators annihilating spin polarons and a pair of operators creating spin polarons at pairs of nearest neighbor sites. The appearance of such terms may be understood by means of a simplest example depicted in Fig.1(a). A slanted cross in Fig.1(a) represents a spin turned upside down in comparison with the Néel state, which is a defect in the initial spin background and will be called a magnon from now onward. A block square denotes a site occupied by a spin pointing in the same direction as in the initial Néel state. The left and the right part of Fig.1(a) represent

two holes created in the AF (Néel) background on the left and right pairs of sites, respectively. In order to clarify the meaning of symbols used in Fig.1 we present the same states in Fig.2(a)-(c) in an explicit way. A wavy line represents a frustrated link for which the static contribution to the exchange energy, which is diagonal in the basis of spin up-down states, is raised in comparison with the Néel state. The states depicted in the left and right parts of Fig.1(a) and Figures 2 (a) and (c) are components of two different bipolarons $|\Psi_{i,j}\rangle$ created at two different pairs of sites i, j. In both cases, by hopping outward the accompanying hole, the hole at the central site creates a state depicted in the middle of Fig.1(a) and in Fig.2(b) which is simultaneously the component of those two different bipolarons.
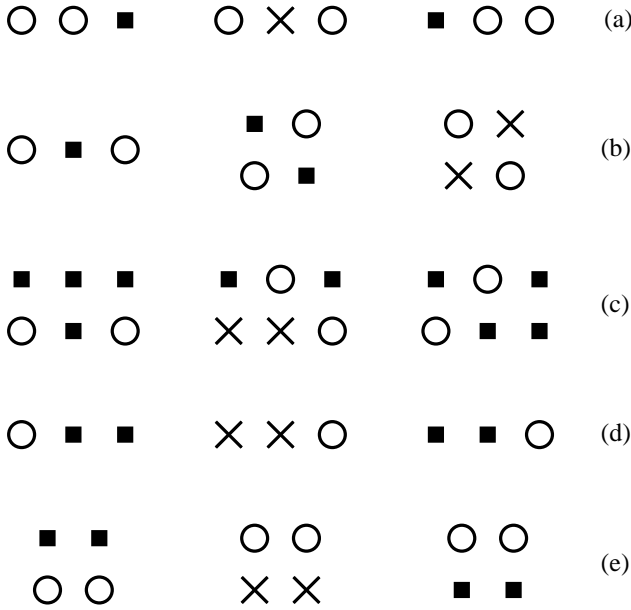

FIG. 1. Schematic representation of some processes contributing to the Hamiltonian and the overlap operator.

Equivalence between components of bipolarons created at different sites gives rise to the overlap between them. By further hopping, holes create more equivalent states and the total overlap between bipolarons created on nearest neighbor sites may be written as a sum,

$$\omega = - \sum_{\mu=0,\nu=1} (z-1)^{\mu+\nu-1}\alpha_{\mu,\nu}\alpha_{\mu+1,\nu-1}, \quad (4)$$

where $z = 4$ is the coordination number and the minus sign is a matter of convention. Analogously, to each string state of arbitrary length, which consists of aligned magnons and holes at both end-points, may be attributed overlap between bipolarons created at outer pairs of sites. In the language of the second quantization the overlap between bipolarons may be represented in terms of a pair of operators annihilating spin polarons and a pair creating them, as for example,

$$\delta\hat{O} = \omega \sum_i h^\dagger_{i+\hat{\mathbf{x}}} h^\dagger_i h_i h_{i-\hat{\mathbf{x}}} \quad (5)$$

in the previously discussed case, where $\hat{O}$ is an operator representing the overlap.
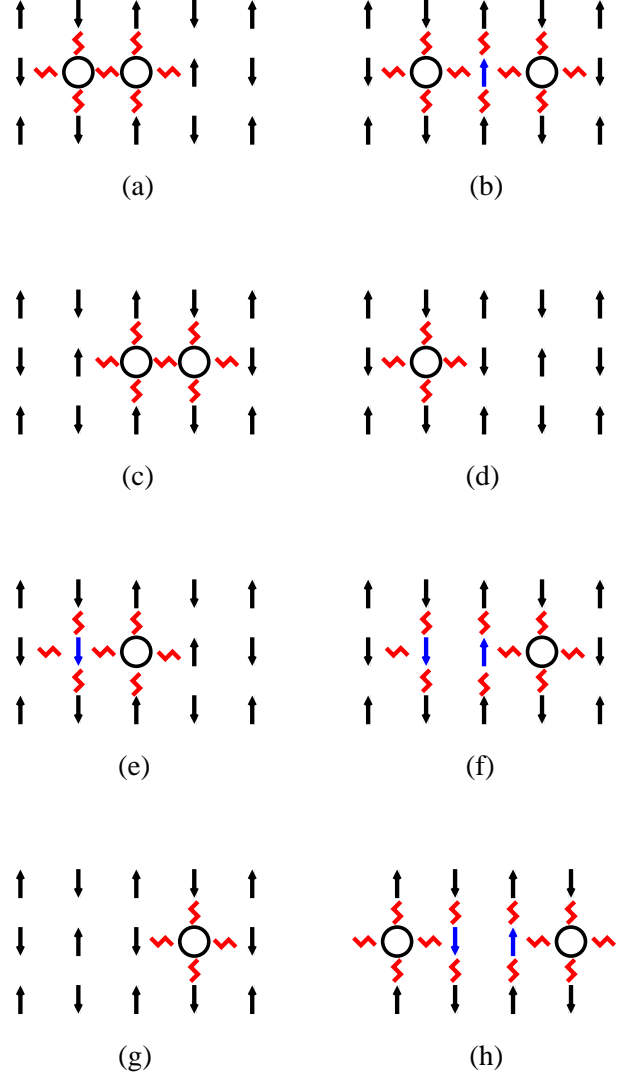

FIG. 2. Explicit representation of some states schematically depicted in Fig.1.

It turns out that each non-trivial contribution to the overlap operator brings about a new contribution to the effective Hamiltonian. By applying the kinetic energy term to the state represented in the middle of Fig. 1(a) and Fig. 2 (b) which is a component of the bipolaron created at a pair of sites represented by circles in the left part of Fig.1(a), the left hole may be shifted to the central site and a state represented by the right part of Fig.1(a) or Fig.2(c) will be obtained, which means that spin polarons created at different pairs of sites marked by circles in outer parts of Fig.1(a) are coupled by the Hamiltonian.

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That coupling was neglected, when we were solving the trial Hamiltonian, because holes created at a pair of nearest neighbor sites were prohibited to retrace each other. Longer strings obtained by further hopping of the right hole may be also involved in analogous processes and the related contribution to the Hamiltonian is,

$$\delta\hat{H} = -t \sum_{\mu=1} (z-1)^{\mu-1} \alpha_{0,\mu} \alpha_{0,\mu-1} \sum_i h_{i+\hat{\mathbf{x}}}^\dagger h_i^\dagger h_i h_{i-\hat{\mathbf{x}}}. \quad (6)$$

Longer strings are crucial to effectiveness, in lowering the energy, of processes driven by the kinetic term in the Hamiltonian. They have been neglected in previous analyses by different authors which lead them to an incorrect conclusion that the collective motion of a hole pair connected by a string can not bring about pairing. We will later discuss that issue. At this stage of our considerations it is necessary to mention that the contributions to the energy which are brought about by the processes included in the trial Hamiltonian are incorporated into the eigenenergies of the polaron E_1 and the bipolaron E_2 and appear in the effective Hamiltonian as diagonal terms

$$\delta\hat{H} = E_1 \sum_i h_i^\dagger h_i \quad (7)$$

and

$$\delta\hat{H} = (E_2 - 2E_1) \sum_{i,\delta} h_{i+\delta}^\dagger h_i^\dagger h_i h_{i+\delta}, \quad (8)$$

where δ denotes links to nearest neighbors of i. Since the absolute value of amplitudes α_μ, $\alpha_{\mu,\nu}$ declines, when the length of strings μ or $\mu+\nu$ grows, only short string states may bring about considerable contributions to the effective Hamiltonian. This remark concerns only the shortest strings which are involved in a process of a given type as in the Fig.1(a). As we have mentioned before, also longer strings obtained by further hopping of holes in the state presented in Fig.2(b) may take part in an analogous process. Since the number of such strings grows exponentially with the length, their contributions should be also taken into account as we did in (5) and (6). On the other hand, in this paper the analysis of processes is restricted to shortest strings (of maximal length of 2 lattice spacings) which are involved in a given process and 'initiate' the whole family of longer strings that may also take part in it. We apply an obvious defining convention that the string length in these units is equal to the number of magnons created by hopping holes, which means that the maximal distance between holes connected by a string of length 2 is 3 lattice spacings. Restricting our calculation to processes which involve strings with the minimal length not longer than 2 lattice spacings needs some justification. By solving the Schrödinger equation determining the shape of spin polarons we deduce that the weight of a string state of length 3 is already smaller at least by one order of magnitude than the weight of states representing bare holes created in the Néel state

and drops faster with the increasing length. Thus, we immediately realize that the weight of shortest strings involved in a given process basically determines the order of magnitude of its amplitude which may be also confirmed by explicit evaluation of formulas like the sums (5) and (6). In addition, results of experiments with neutron scattering performed for $La_{2-x}Sr_xCuO_4$[16] suggest that the AF correlation length in the cuprates follows the the mean hole distance which allows us to make an estimate that the spin polaron approach to pairing in weakly doped AF will provide reasonable results for the doping parameter $\delta \leq 1/9$ for which the AF correlation length is longer than the average distance between the holes that form the spin bipolaron, which we estimate to be about 2-3 distances between copper atoms. The applicability of the string approach to the whole underdoped region, for example for the doping parameter up to the value 1/4 starts to be questionable because at that value the AF correlation length is surely not higher than 2 distances between copper atoms. Thus we may asses the validity of the spin polaron method for description of pairing for the doping parameter higher than $\delta \simeq 1/9$ only by comparing with the results of numerical calculations.

The hypothesis about the tight relation between AF correlations and SC in the cuprates has been recently confirmed once again by observing the coexistence of the AF order with the SC state in $YBa_2Cu_3O_{6.5}$[17]. That observation suggests that the region where the spin polaron approach is applicable may indeed be wider.

In a recent preprint an absence of in plane hole ordering and the homogeneity of holes in the superconducting compound $La_2CuO_{4+\delta}$ was observed above T_c by means of anomalous x-ray scattering at the oxygen K edge[18]. On the other hand the problem of phase separation in the t-J model is a delicate issue. Emery et $al.$ suggested that the phase separation in the 2D t-J occurs at all interaction strengths[19]. Results of a high-temperature expansion (HTE)[20] and of a Green's function Monte Carlo (GMFC) calculation[21] indicate that the t-J model does not phase separate for the values of the ratio J/t relevant for HTSC. These conclusions were questioned in a series of papers by different authors[22,23] who found phase separation at half-filling for all values of the interaction-strength J/t. Their findings are little surprising because in a previous paper[7] they showed that binding of holes occurs above a certain finite value of the ratio J/t. Our analysis of the 1D t-J model in the staggered magnetic field introduced in order to mimic the physics in 2D suggests that large clusters of holes are heavy objects and that their formation will mean a great loss of the kinetic energy which makes the phase separation to be unlikely at low values of the parameter J/t[24]. In addition, recent DMRG calculations[11,25] indicate that the phase separation occurs in the t-J model for $J/t \geq 1.4$ which roughly agrees with the results of HTE. On the other hand, in the physically relevant region of parameters stripes are observed in results of DMRG calculations. Notwithstanding the outcome of the discussion about the robustness

of phase separation in the *t-J* model at half-filling for the values of the parameter J/t which are relevant from the physical point of view, it is clear that this phenomenon is very sensitive to the Coulomb repulsion. This interaction does not spoil the mechanism of pairing because the binding holes are located at longer distances. Even if the effects related to Coulomb repulsion are neglected and even if the statement about the phase separation in the *t-J* model at half-filling at all interaction strengths is taken seriously, there seems to exist a region near the doping level about $\delta \simeq 1/9$ where the system is not phase separated for physically relevant values of the interaction strength, and the discussed in this paper formulation of the spin polaron approach is applicable. On the other hand it is clear that the issue of phase separation needs further analysis in future, also in the framework of the string approach.

Less controversial are experimental[26] and theoretical[11,25] findings that stripes form in doped antiferromagnets. The physics of the stripe phase like the physics of binding is determined by the balance between the kinetic and the exchange energy. Since the domains between stripes are antiferromagnetically ordered the methodology of spin polaron approach may be applied to the analysis of the stripe phase[27,28]. It is unlikely that the formation of stripes is a driving mechanism for superconductivity but pairing may in principle also take place in the stripy background. The analysis of this phenomenon by means of the spin polaron method may be done but is beyond the scope of this paper.

While constructing the effective Hamiltonian we not only take into account processes, which were omitted when the trial Hamiltonian was solved, but also make some amendments to approximations we made previously. Since the wave function of a spin multi-polaron representing holes created at a distance longer than one lattice spacing is approximated by the product of wave functions, some corrections are necessary. By considering that kind of products we tacitly assumed that both holes in the left part of Fig.1(b) may simultaneously jump on the middle site. That artificial state should be removed, which gives rise to a necessary correction in the normalization condition for a pair of spin polarons created at sites marked by empty circles in the left part of Fig.1(b) and an additional term in the operator representing overlap between pairs of polarons. Also an appropriate correction to the eigenenergies of single polarons should be made for polarons created at such a small distance, because the obvious restriction on possibility of hopping of holes on top of each other was neglected when we solved the Schrödinger equation defining single polaron states, which means that some spurious processes were taken into account during the evaluation of the kinetic energy. There are some more non-existing states which we artificially incorporated into the calculation, by assuming that the wave function of spin polarons created at the distance higher than one lattice spacing may be approximated by a product of wave-functions for separated polarons. For

example, the left hole in the left part of Fig.1(b) can not move to the right site occupied by the second hole. Similar restrictions concern two holes and polarons created at opposite ends of the cell diagonal, as in the middle panel of Fig.1(b), and should bring about appropriate corrections both to the operator which represents the overlap between polarons and to the Hamiltonian formulated in the polaron language. In addition, the same state in the right panel of Fig.1(b) may be obtained in two different ways when the upper hole in the middle part of Fig.1(b) hops once vertically or horizontally while the lower hole hops in the opposite way, which gives rise to an additional contribution to the normalization condition for the wave function of two polarons occupying opposite corners of an elementary cell. By means of a detailed analysis of string states we may find more examples of overlap between pairs of polarons created at different pairs of sites and more contributions to the Hamiltonian related to the kinetic energy. By hopping twice, first to the right and next upward, the left hole in the left part of Fig.1(c) may transform the state without magnons in the vicinity of holes into a state represented by the middle part of Fig.1(c). The same result may be achieved if the left hole in the right diagram in Fig.1(c) hops twice to the right, which means that components of two different pairs of polarons localized at sites represented by circles in outer parts of Fig.1(c) are identical and that the wave functions of different pairs of polarons overlap. In addition, a shift of one of two holes in the middle diagram to the site occupied by the central magnon, caused by the application of the kinetic term in the TJM transforms a component of a wave function for one pair of polarons into the component of another pair, which means that the effective Hamiltonian couples different pairs of polarons. Until now, we have considered only two categories of contributions to the Hamiltonian expressed in the basis of spin polarons, terms which represent eigenenergies of spin polarons, and terms related to the fast motion of holes, with the rate $\sim t$, or in other words matrix elements of the Hamiltonian which represent coupling between spin polarons by the hopping part of the TJM. Different spin polaron states may be also coupled by terms in the TJM related to the magnetic exchange. Their action, which occurs at a slower rate $\sim J$, turns upside down anti-parallel spins at nearest neighbor sites. That coupling was neglected when the spin polaron basis was constructed. Fig.1(d) shows a most obvious process, which gives rise to coherent propagation of a single hole in the AF medium. The left diagram represents a hole created in the AF spin background. This state is also a component of a spin polaron created at the left site. Another component of that polaron depicted in the middle diagram will be obtained if the hole hops twice from the left site to the right site. Two magnons created in this way may be annihilated if the transversal part of the Heisenberg model is applied to the state represented by the middle part of Fig.1(d). The new state, which is a component of the spin polaron localized at the right site, is repre-

sented by the right diagram in Fig.1(d). Four Figures 2(d)-(g) represent the same sequence: the initial state, two intermediate states obtained by hopping of the hole and the final configuration in which two shifted spins has been swapped. The magnetic exchange may also couple a spin polaron representing two holes attached by strings to a pair of nearest neighbor sites with another spin bipolaron or a pair of separated spin polarons. A process depicted by Fig.1(e) may be analyzed in a way similar to that which was applied in the case of the process represented by Fig.1(d). The intermediate state in the middle of Fig.1(e) is a component of a spin bipolaron localized at a lower part of sites marked by circles in the left diagram. Annihilation of spin defects, or in other words magnons, by the transversal part of the Heisenberg model gives rise to the creation of a state represented by the right diagram. That state is a component of the spin bipolaron created at the upper pair of sites, which means that the spin bipolaron is effectively shifted upward by one lattice spacing. If holes initially created at a lower pair of sites do not hop in the same direction, an analogous process will transform the spin bipolaron into a pair of separated spin polarons. The process depicted in Fig.1(d) is of paramount importance for the selection of the symmetry of the bound state of two holes created in an AF[6], because it lowers the energy of the $d_{x^2-y^2}$-wave state and raises the energy of the p-wave state, while the rest of low order processes which involve only spin bipolarons is neutral. The proximity between the energies of lowest states which show these symmetries has been recently confirmed by an exact diagonalization performed for a relatively large cluster[9]. We expect that the preference for the $d_{x^2-y^2}$-wave symmetry will prevail in the hypothetical SC state, which may emerge after polaron pairs condense.

Some additional amendments to terms in the Hamiltonian which are diagonal in the spin-polaron representation are necessary. For example, our analysis should also take into account that holes initially created at sites which are not nearest neighbor sites, may gain some potential energy by lowering the number of broken bonds, when they occupy such a pair after they made a few hops. We may meet such a situation if holes have been initially created at the Manhattan distance of two lattice spacings like in the middle part of Fig.1(b). After a hop of a hole toward its companion the number of broken bonds is lower by one than after a single hop of one of two holes initially created at a longer distance. The discussion of quantum fluctuations in the AF state which lower the energy of the ground state of the Heisenberg model in comparison with the energy of the Néel state that is the groundstate of the Ising model is also incorporated into our calculation. In the lowest order of the perturbation theory such fluctuation represent pairs of magnons created at NN sites in the Néel state and change the energy by the amount $-J/12$ for each link.

At the chosen level of accuracy there are altogether 14 different contributions to the overlap operator and 58

to the Hamiltonian, which may be classified according to processes that give rise to them and the positions of involved polarons. The physical picture which underlies the principle according to which the Hamiltonian is constructed is based on the assumption that the dynamics of holes should not destroy local AF correlations. For example in the process depicted in Fig.1(a) and Figures 2(a)-(c) the defects in the spin structure created by the motion of the right hole are annihilated by the subsequent hopping of the left hole. Thus, by the exchange of magnons forming a string which connects two holes, hole pairs initially created at NN sites avoid confinement. The process depicted in Fig.1(d) and Figures 2(d)-(g) which deconfines a single hole may be interpreted as cutting of the string formed by magnons attached to the initial site, by the transversal part of the exchange term in the Hamiltonian.

Without dwelling more upon details we present now the form of the effective Hamiltonian expressed in terms of operators h_i and $h_i^\dagger$ annihilating and creating spin polarons.

$$\hat{H} - \mu\hat{N} = (E_1 - \mu)\sum_i h_i^\dagger h_i + h_1 \sum_{i,\delta,\delta';\ \delta'\neq-\delta} h_{i+\delta+\delta'}^\dagger h_i$$

$$+(E_2/2 - E_1 + u_1)\sum_{i,\delta} h_i^\dagger h_{i+\delta}^\dagger h_{i+\delta} h_i$$

$$+u_2 \sum_{i,\delta,\delta';\ \delta'\neq-\delta} h_i^\dagger h_{i+\delta+\delta'}^\dagger h_{i+\delta+\delta'} h_i$$

$$+u_3 \sum_{i,\delta,\delta';\ \delta'\perp\delta} h_i^\dagger h_{i+\delta+\delta'}^\dagger h_{i+\delta+\delta'} h_i$$

$$+u_4 \sum_{i,\delta,\delta',\delta'';\ \delta'\neq-\delta,\delta''\neq-\delta'} h_i^\dagger h_{i+\delta+\delta'+\delta''}^\dagger h_{i+\delta+\delta'+\delta''} h_i$$

$$+s_1 \sum_{i,\delta,\delta';\ \delta'\neq-\delta} h_{i+\delta+\delta'}^\dagger h_{i+\delta}^\dagger h_{i+\delta} h_i$$

$$+s_2 \sum_{i,\delta,\delta',\delta'';\ \delta'\neq-\delta,\delta''\neq-\delta'} h_{i+\delta+\delta'}^\dagger h_{i+\delta+\delta'+\delta''}^\dagger h_{i+\delta} h_i$$

$$+s_3 \sum_{i,\delta,\delta';\ \delta'\perp\delta} [(h_i^\dagger h_{i+\delta+\delta'}^\dagger h_{i+2\delta} h_i + H.c.)$$

$$+h_i^\dagger h_{i+\delta+\delta'}^\dagger h_{i+\delta-\delta'} h_i]$$

$$+s_4 \sum_{i,\delta,\delta',\delta'';\ \delta'\neq-\delta,\delta''\neq-\delta'} (h_i^\dagger h_{i+\delta+\delta'+\delta''}^\dagger h_{i+\delta} h_i + H.c.)$$

$$+s_5 \sum_{i,\delta,\delta';\ \delta'\perp\delta} h_i^\dagger h_{i+\delta'}^\dagger h_{i+\delta} h_i$$

$$+s_6 \sum_{i,\delta,\delta',\delta'';\ \delta'\neq\delta,\delta''\neq-\delta} (h_{i+\delta+\delta''}^\dagger h_{i+\delta'}^\dagger h_{i+\delta} h_i + H.c.)$$

$$+s_7 \sum_{i,\delta,\delta';\ \delta'\perp\delta} h_{i+\delta+\delta'}^\dagger h_{i+\delta'}^\dagger h_{i+\delta} h_i \qquad (9)$$

Parameters which appear in this effective Hamiltonian are functions of E_1, E_2, μ, t, J and amplitudes α and include at once contributions from many different types of processes. An important remark which we should also

make is that the highest value for experimentally relevant ratios J/t has a parameter related to the motion as a whole of strings connecting a pair of holes, example of which is depicted in Fig 1(a). That type of caterpillar-like motion is so effective in lowering of the total energy because by expanding at one end and shrinking at the other, the whole string may move freely, while the number of magnetic defects is kept low. Only the kinetic term in the Hamiltonian is involved in that movement and the term related to the magnetic exchange does not have to intervene. Thus the gain in the energy is mainly due to lowering of the kinetic energy.

It is widely believed[30−32] that the motion of the hole pair is frustrated and can not bring about lowering of the total energy and binding or pairing. Already the analysis of hole binding[6] provided arguments that such an opinion is not correct. The notion of frustration was used in literature to describe the fact that effective hopping of the hole pair occupying NN sites, to nearest links which are parallel and perpendicular to the link at ends of which the holes have been initially located, produces effective hopping integrals with the same positive sign, which is not very convenient in terms of lowering the kinetic energy, but does not change a generally applying rule that a mobile quantum object has lower energy than an immobile one. We have previously shown, that the motion of a hole pair connected by a string formed by defects in the AF spin structure may give rise to formation of bound states with $d_{x^2-y^2}$ and p-wave symmetries, which agrees with results of numerical analyses including a recent work[9] performed for a relative large cluster consisting of 32 sites. Also the energetic hierarchy of two-hole states representing symmetries and wave vectors allowed by the geometry of the 4×4 cluster observed by Hasegawa and Poilblanc[33] in the results of the exact diagonalization has been reproduced by means of the spin polaron approach. Since the interaction between spin polarons mediated by the processes related to the motion of the string connecting two holes is dominating, the agreement between numerical and analytical analyses indicates that the spin polaron approach properly takes into account such effects. Arguments against the kinetic energy driven mechanism of binding in doped AF are based on the large d expansion[32]. A single hole created in the Néel background may lower the energy by virtual hopping to NN sites. If two holes occupy NN sites, the hopping of each hole in one direction is blocked and the energy is raised by the amount $2t^2/Jd$ in comparison with the energy of two separate holes. On the other hand if holes are created at NN sites one spoiled AF link is saved and a negative contribution $-J/2$ to the total energy is generated. In the first order of the $1/d$ expansion, the propagation of a hole pair occupying NN sites mediated by the process represented by Fig.1(a) may only compensate the loss in the energy related to the blocking effect and no net gain in the energy related to the hole-pair kinetics is observed. That picture changes qualitatively in lower dimensions for $t \gg J$. The energy scale $\sim t^2/J(d-1)$ dominates the

scale $\sim J(d-1)$ and the energetical cost related to creation of longer strings similar to the state represented by Fig.2(h) is relatively lower. In addition, there is no blocking effect in the case of strings with at least one magnon. In simple words, holes at ends of longer strings can hop at least once in all directions without disturbing each other. All this makes the creep of strings more effective in lowering the energy. In 2D any simple calculation based on the $1/d$ expansion or an approach limited to a small basis of states related to short strings will not provide reliable results. During the construction of the spin polaron and the bipolaron the important contribution to the energy from incoherent motion in the potential wells and longer strings has also been taken into account. The energy of the spin bipolaron by construction contains contributions related to saving spoiled AF links and mutual restricting the freedom of motion by two holes which oscillate chaotically around a pair of NN sites where they have been initially created. It turns out that for physically relevant range of parameters these two effects almost compensate each other and the eigenenergy of the localized spin bipolaron is roughly twice the energy of a localized polaron. Thus, truly kinetic effects related to motion of the center of mass of a hole pair connected by a string bring about a net gain in the kinetic and total energy. In the effective Hamiltonian these effects are represented by terms related to hopping of bipolarons. The difference between behavior in low and high dimensions may be associated to the change in the relation between the energy scales $J(d-1)$ and $t^2/J(d-1)$ and to the related fact that the creation of longer strings is not so costly in lower dimensions.

If phase separation indeed takes place at half filling the Coulomb repulsion between holes at NN sites may prevent that effect, but will not influence pairing so much, because the total probability that holes which form a spin bipolaron are at a longer distance is much higher than they occupy NN sites. A detailed analysis of effects related to the Coulomb repulsion is beyond the scope of this paper.

The wave functions of spin polarons are not orthonormal and the operator $\hat{O}$ representing overlap between them takes an unconventional form,

$$
\begin{aligned}
\hat{O} = 1 &+ d_1 \sum_{i,\delta,\delta';\, \delta'\neq-\delta} h_i^\dagger h_{i+\delta+\delta'}^\dagger h_{i+\delta+\delta'} h_i \\
&+ d_2 \sum_{i,\delta,\delta';\, \delta'\perp\delta} h_i^\dagger h_{i+\delta+\delta'}^\dagger h_{i+\delta+\delta'} h_i \\
&+ o_1 \sum_{i,\delta,\delta';\, \delta'\neq-\delta} h_{i+\delta+\delta'}^\dagger h_{i+\delta}^\dagger h_{i+\delta} h_i \\
&+ o_2 \sum_{i,\delta,\delta',\delta'';\, \delta'\neq-\delta,\delta''\neq-\delta'} h_{i+\delta+\delta'}^\dagger h_{i+\delta+\delta'+\delta''}^\dagger h_{i+\delta} h_i \\
&+ o_3 \sum_{i,\delta,\delta';\, \delta'\perp\delta} [(h_i^\dagger h_{i+\delta+\delta'}^\dagger h_{i+2\delta} h_i + H.c.) \\
&+ h_i^\dagger h_{i+\delta+\delta'}^\dagger h_{i+\delta-\delta'} h_i].
\end{aligned}
\tag{10}
$$

Since the explicit formulas for the parameters of the Hamiltonian and the overlap operator are rather lengthy, they will be presented in the Appendix.

IV. PAIRING VERSUS PSEUDOGAP PHASE IN DOPED ANTIFERROMAGNETS

The distance between two holes which form a bound state in the AF background is few lattice spacings[6] and it is natural to analyze their paring in the real space. That approach is suitable for superconductors with the short coherence length. For the sake of simplicity we concentrate on anomalous Green's functions $\mathcal{F}(i, \tau; i', \tau')$,

$$\mathcal{F}(i, \tau; i', \tau') = \langle T_\tau h_i(\tau) h_{i'}(\tau') \rangle, \qquad (11)$$

which represent a pair of spin polarons simultaneously annihilated at a pair of sites i, i' located at the distance not longer than 3 lattice spacings. The rest of anomalous Green's functions which corresponds to longer distances is neglected. That simplification will be justified by showing that $\mathcal{F}(i, \tau; i', \tau')$ decreases fast with the distance between i and i'. Our intention is to reproduce the results of the recent numerical calculation performed by Sorella and collaborators[1] by means of numerical methods. Since they observe pairing correlations at some pairs of nearby sites we may also define the order parameter in the real space for a few short distances. Since attraction between holes is strongest in the $d_{x^2-y^2}$-wave channel we shall for simplicity discuss pairing only of that symmetry. Possible symmetries of the order parameter are determined by irreducible representations of the point group C_{4v}. The order parameter which is a singlet may transform according to one dimensional representations s, $d_{x^2-y^2}$, d_{xy} and g, while the triplet order parameter corresponds to the two dimensional representation p. The pairing at the distance of 1, 2 or 3 lattice spacings may in principle realize the symmetries s, $d_{x^2-y^2}$ and p. Scattering of a hole pair mediated by the process represented by Fig.1(a) and similar caterpillar-like motion of longer strings analogous to the object depicted in Fig.2(h), constitutes the strongest interaction in the Hamiltonian, which determines the dominating symmetry of pairing. This property was already noticed when we discussed binding[6]. That kind of interaction is attractive in the $d_{x^2-y^2}$ and p-wave channels and repulsive in the s-wave channel. Another term in the Hamiltonian related to the process depicted in Fig.1(e) favors $d_{x^2-y^2}$ and suppresses p-wave pairing. Therefore, the dominating terms in the order parameter will have $d_{x^2-y^2}$ symmetry. Interactions which involve holes at slightly longer distances are also relevant. If we restrict pairing in the real space to distances up to 3 lattice spacings, the $d_{x^2-y^2}$ symmetry will generate in the order parameter three independent harmonics $D_{\mathbf{k}}^{(1,0)}$, $D_{\mathbf{k}}^{(2,1)}$ and $D_{\mathbf{k}}^{(3,0)}$ defined in the Appendix. Necessity to apply a multi-dimensional non-monotonic order parameter was recently suggested

after analysis of results of some experiments with Raman scattering performed for electron doped cuprates[34]. The order parameter representing pairing of holes at the distance $\sqrt{2}$ may transform according to representations s, d_{xy} and p, while for the paring at the distance $\sqrt{5}$ according to the representations s, $d_{x^2-y^2}$, d_{xy}, g and p. In a full analysis of pairing in the real space at distances not longer than 3 lattice spacings we should in principle consider a 24 dimensional order parameter, which is much beyond the scope of this paper, and we will concentrate only on the dominating pairing in the $d_{x^2-y^2}$-wave channel.

We assume that the anomalous Green's function is translationally invariant in space and time,

$$\mathcal{F}_e(\mathbf{x}, \tau) = \langle T_\tau h_{i+\mathbf{x}}(\tau' + \tau) h_i(\tau') \rangle, \qquad (12)$$

and that i in the previous definition belongs to the even sublattice. A relevant order parameter in the real space is defined as,

$$\Delta_{\mathbf{x}} = \mathcal{F}_e(\mathbf{x}, 0^+). \qquad (13)$$

By proceeding in a standard way we derive HF equations for the SC order parameter in which vertex corrections have been neglected. Since retardation effects related to the exchange of magnons have been already taken into account during the derivation of the effective Hamiltonian, the application of the weak coupling approach seems to be appropriate. For the sake of brevity we shall present only in the Appendix the difference between the grand canonical potential in the superconducting and the normal state which may be reconstructed from the equations for the order parameter. The chemical potential applied in this formalism refers to the number of holes $\hat{N}$ which is given by the formula,

$$\hat{N} = \sum_i h_i^\dagger h_i + 2(\hat{O} - 1), \qquad (14)$$

that within the HF approximation may be written at $T = 0$ as

$$\delta = \frac{1}{N} \sum_{\mathbf{k}} (1 - \frac{\xi_{\mathbf{k}}}{E_{\mathbf{k}}})/2 - 8(o_1 - o_2)\Delta_{\hat{\mathbf{e}}_x}^2, \qquad (15)$$

where

$$\delta = \langle \hat{N} \rangle / N. \qquad (16)$$

Quasiparticle energies $\xi_{\mathbf{k}}$ and $E_{\mathbf{k}}$ in the normal and SC state are defined in the Appendix. Since we deal with a two-dimensional (2D) system where fluctuations are strong at finite temperatures and destroy the long range order we perform the analysis only at $T = 0$.

$o_1 - o_2$ turns out to be negative. Thus it is clear that Eq.15 will enforce disappearance of the SC order parameter when the number of holes decreases. Fig.3 depicts anomalous Greens function that represent the SC order

parameter related to pairs of spin polarons condensing on some nearest pairs of sites in the real space obtained within the weak coupling approximation applied to the effective Hamiltonian for $J/t = 0.33$.

Numerical analyses of the TJM indicate that the AF correlations decrease with doping and that the correlation length becomes comparable to two or even one lattice spacing, when the doping exceeds 20% which agrees with the phenomenology of the cuprates. Since the spin-polaron approach is based on the assumption that the polaron radius is smaller than the correlation length, we can not expect that our analysis will give any reasonable solutions to the problem of pairing in doped AF for the values of the doping parameter δ right to the vertical line drawn in Fig.3 at $\delta = 0.2$. On the other hand the agreement for the underdoped system between the analytical approach and numerical results of Sorella and collaborators[1] is reasonable at the left side of the vertical line which exceeds our earlier expectations that the string approach should provide correct results for doping levels δ below 1/9. Robustness of the SC solution up to the doping level $\delta = 0.9$ indicates that the disappearance of SC in the overdoped region should not be attributed merely to the change in the band-filling, but to the reconstruction of the effective interaction which mediates pairing. The low energy Hamiltonian for spin polarons which we use is not filling-dependent and does not take into account effects related to the degradation of spin polarons at higher doping levels.
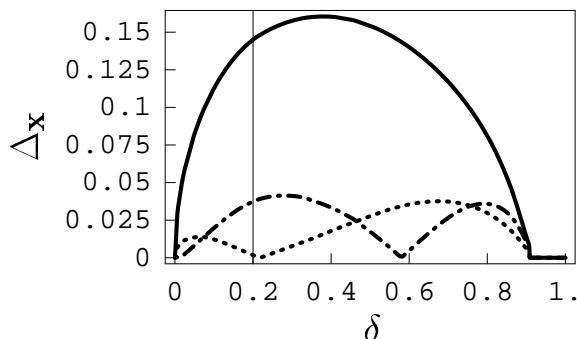

FIG. 3. Anomalous Green's functions $\Delta_{\mathbf{x}}$ which represent pairs of spin polarons condensing at the distance of 1 lattice spacing (continuos line), $\sqrt{5}$ lattice spacings (dotted line) and 3 lattice spacings (dash-dotted line).

Our calculation also demonstrates that the energetic gain is not due to minimization of the number of broken bonds in the AF state if holes reside on a pair of nearest neighbor sites, but pairing actually occurs because by formation of spin bipolarons, the magnetic and kinetic components of the energy may be simultaneously lowered. Since $t \gg J$, lowering of the kinetic energy plays a leading role in pairing, which confirms recent experimental observations[35] that the spectral weight in the plots of optical conductivity is shifted toward lower energies below T_c and in the pseudogap region. We also observe that

the SC order parameter vanishes in the limit of low hole doping, which may be attributed to emptying the spin polaron band and approaching the Mott insulator (MI) phase in the nominally half-filled system. A rigid band picture which may be associated with propagating spin polarons has been recently observed by means of ARPES measurements in the Na-doped $Ca_2Cu0_2Cl_2$ by Shen, Takagi and collaborators[36,37]. The only effect which has doping up to the level above 10% is the shift of the chemical potential. In addition, some recent measurements of optical conductivity in underdoped cuprates performed by Basov and collaborators[38] indicate that approaching the insulator regime in this system may be attributed to localization effects in an band which is emptied.

The vanishing of the SC energy gap related to the coherent SC state does not necessarily mean that the underdoped AF should reveal features of an ordinary Fermi liquid-like normal state, because the system of freely propagating spin polarons becomes unstable against formation of bipolarons which brings about opening of the a pseudogap in the spectral function of a single quasiparticle. An earlier analysis[14] together with results presented in this paper and some numerical calculations[8,9] demonstrate that the binding energy of a hole pair in the AF medium, which according to our scenario should be the energy scale of the pseudogap near half-filling is a bigger fraction of J than the SC energy gap at optimal doping, which is in rough agreement with the phenomenology of the cuprates.

There exists a direct relation between formation of bound hole-pairs of $d_{x^2-y^2}$-wave symmetry and existence of current-current correlations that form the pattern of a staggered flux[39−41], which makes a connection between the local pair scenario for the pseudogap phase and the idea of a hidden order in the d-density wave phase[42]. Some earlier analyses also suggest that the the appearance of the stripe phase in weakly doped AF is very likely, because gains achieved by formation of stripes and spin polarons[27] or bipolarons[29] are similar. Localization effects which should accompany a transition to MHI in the limit of low doping and the intrinsic disorder[43] which is a characteristic feature of the cuprates may also additionally complicate the physical picture of the relation between the superconducting state and the pseudogap phase.

V. CONCLUSIONS

The analysis presented in this paper allows to identify spin fluctuations which mediate pairing. It turns out that the coherent propagation of magnons which takes the form of spin waves is not relevant to pairing. A process which gives rise to magnon propagation has been depicted in Fig.4.

FIG. 4. A process responsible for spin wave propagation.

A magnon at the left site in the left panel will be effectively shifted to the right site in the right panel if the transverse part of the Heisenberg model is applied to the state depicted in the middle panel which represents the magnon and an additional spin fluctuation, included in an oval, that exists in the ground state of the 2D AF. Inclusion of such processes into considerations does not influence the results, which proves that the standard propagation of spin waves does not play a crucial role in pairing. Emission of spin fluctuation by a hopping hole, which are later annihilated by the second hole that retraces the first hole has a quite different nature and is a dominating factor in pairing. On the other hand, the coupling between the spin degrees of freedom represented by independently propagating magnons, and the charge which may be attributed to holes, gives rise to unconventional excitations in doped AF for example with the charge $Q = 1$ and spin $S_z = 3/2$ which have been observed in the numerical calculation by Hasegawa and Poilblanc[33]. Such a quasiparticle may be interpreted as a bound state of the excess magnon and the hole. It is possible to analyze that effect in the framework of the spin polaron approach. However, interaction between independently propagating spin waves and holes does not influence the properties of the paired state and that kind of coupling has been neglected in this paper. A general statement that pairing in the region of small doping is driven by spin fluctuations is rather an oversimplification. Formation of spin polarons and bipolarons in the locally AF background is actually a complex process of lowering simultaneously the exchange energy and the kinetic energy.

The form of the effective Hamiltonian (9) indicates that the pairing mechanism is essentially nonretarded and effective interactions have a short range which agrees with conclusions drawn from the universal trends observed for the cuprates in the dependence of T_c on the hole and condensate density[44].

According to our scenario, phase fluctuations may play a lesser role in formation of the pseudogap than it was earlier suggested[45] because even in the mean field approximation the order parameter for SC vanishes in the limit of weak doping, which follows directly from the relation between the chemical potential, number of holes and the SC order parameter. It is, however, clear that fluctuation effects are visible in all extreme type II superconductors with a short coherence length and that they play an essential role in the thermodynamic behavior. For example, the measured thermodynamic properties of cuprate superconductors reveal consistency with the critical behavior of the 3D XY model[46]. On the other hand the disproportion between the vanishing gap function in the limit of low doping and the finite energy of

the hole-pair binding is more fundamental to the spectral properties of a single quasiparticle and the formation of the pseudogap. Notwithstanding that the Hamiltonian (9) is exclusively written in terms of fermionic operators it is clear that it will reveal some features of the local pair physics[47]. According to some earlier estimations[6], in the case of two holes created in the quantum AF about 70% of the weight in the $d_{x^2-y^2}$-wave bound state belongs to the bipolaron wave function which represents two holes connected by strings consisting of magnons. Those strings are pinned to pairs of nearest neighbor sites, which determine the position of bipolarons. It is sufficient to consider only hopping of bipolarons, mediated by shrinking and expanding of strings at opposite ends, to understand the energetical hierarchy of two-hole states that posses s, $d_{x^2-y^2}$ and p symmetries, which indicates that the local pair physics may be relevant in the limit of low doping. On the other hand, a more appropriate way of thinking about the spin polaron Hamiltonian would be from the point of view of a more general boson-fermion model (BFM)[48]. The identification of spin bipolarons with bosons may serve as justification of the BFM, which is widely analyzed in the context of the pseudogap formation. There exist differences between the standard BFM and a version of it which corresponds to the spin polaron Hamiltonian (9) but the basic behavior should be similar in both cases. The main differences are that spin bipolarons (hard-core bosons) occupy links and that sites at ends of such a link can not be occupied by fermions. Fermions (mono-polarons) at nearby but not nearest neighbor sites transform into bosons when they move to NN sites and vice versa. The energy of the boson localized in space is not much different from the energy of two localized fermions and this energy difference is not crucial to pairing. A driving mechanism of effective attraction between fermions and formation of bipolarons (bosons) is the high mobility of the latter. Condensing spin bipolarons predominately contribute to the SC state of a short coherence length.

We can draw an interesting conclusion concerning the pseudogap in doped AF from the comparison of the left panel in Fig.3 with the seemingly useful right panel. If AF spin fluctuations are responsible for pairing, which we believe is generally true, the mechanism of attraction between quasiparticles will become less effective when doping increases and our model becomes irrelevant right to the vertical line in Fig.3. Thus, the fast decrease of T_c with doping observed in real systems and the fast disappearance of the order parameter demonstrated in the numerical analysis should be attributed to diluting of the spin system an disappearance of the driving factor which is identified as AF short range correlations. That remark concerns also the temperature of the crossover to the pseudogap behavior, which decreases with doping already in the underdoped region and somewhere near optimal doping merges with T_c. The lowering of T_c in the underdoped region with the decreasing number of holes should not be attributed to the disappearance of the at-

tractive force between quasiparticles but to emptying the spin polaron band. The later effect does not influence binding of hole pairs which gives rise to pseudogap phenomena. That rough scenario will in reality be modified by dimensionality effects, phase fluctuations, and some other phenomena like tendency toward phase separation and stripe formation. A more detailed analysis of pseudogap formation in the spin polaron model for weakly doped AF in the framework of a method suitable for low density systems, which is the T matrix approach[49] is beyond the scope of this paper.

A phenomenological scenario in which superconductivity is mediated by lowering of the kinetic energy has been suggested by Hirsch[50,51], who introduced the notion of hole undressing. It seems that the same term may be applied to describe physics of spin polaron pairing. Single holes form mono-polarons which are heavy objects because their propagation is mediated by the process represented by Fig.1(d) which involves the action of the exchange term and the effective hopping amplitude is therefore small. Two bound holes may propagate collectively without intervention of the exchange interaction and they behave more like bare undressed holes. This remark agrees with experimental observations that HTSC cuprates reveal transition to a more coherent state as the system becomes SC. Microscopic models analyzed by Hirsch and their physics are quite different from our effective Hamiltonian and the spin polaron scenario. The analysis of these models lead to a conclusion that the undressing scenario may apply only to holes. On the contrary, at the level of the t-J model, the spin polaron scenario is also applicable to electron doped systems in which the physics of doubly occupied sites (particles) is the same as the physics of holes in hole doped systems.

The analysis of pairing in weakly doped AF in terms of bipolaron formation seems to be complementary to the spin fluctuation approach[52] formulated by Pines and collaborators for optimally doped and overdoped systems.

In summary, by constructing an effective Hamiltonian we have identified spin fluctuations which mediate pairing in doped AF as local spin fluctuations which lie on a path connecting two holes. Creep-like motion of the whole object is an effective way of lowering the kinetic energy and the predominant factor which gives rise to pairing. This contradicts previous statements and widespread opinions based on the $1/d$ expansion that the collective motion of two holes in the locally AF background can not effectively lower the energy. The experimental evidence that pairing may be associated with the change in the kinetic energy has been recently found by a second group[53]. These researchers were actually looking for a transfer of spectral weight from lower to higher energies in the pseudogap region, but observed an opposite behavior, which supports the suggestion that the physics of the pseudogap may be also related to binding of holes.

The analysis of the effective Hamiltonian obtained by means of a method which has both a variational and perturbative character reproduces the behavior of the SC order parameter obtained by means of numerical analysis[1] with reasonable accuracy up to the doping level $\delta \approx 0.2$, which exceeds our expectations that the spin polaron method should be valid for $\delta \leq 0.11$. We also provided arguments that even within a most favorable scenario for phase separation, the pairing consistent with the string picture will occur in the region around the doping level $\delta = 1/9$. Data presented in a recent review[54] of numerical approaches to strongly correlated lattice models indicate that pairing correlations are smooth functions of the Manhattan distance which indicates that the physics of strings is visible in these results. Some recent experimental results obtained by measuring optical conductivity[38] and ARPES[36] confirm the relevance of the band scenario at low doping which is consistent with the spin polaron approach.

The strength of the attraction mediated by spin fluctuations decreases with doping and the diminishing AF correlation length. That effect may explain decreasing of the pseudogap with doping and the disappearance of superconductivity in the overdoped region. On the other hand in the underdoped region SC disappears, because the quasiparticle band is emptied, while the density of low energy excitations is still suppressed by formation of bound hole pairs.

We start the Appendix with the presentation of parameters which define the Hamiltonian and the overlap operator in terms of operators creating and annihilating spin polarons

$$h = 2M_{\{(2,0)\}\{(0,0)\}} \tag{17}$$

$$u_1 = J^H_{\{(0,0)\}\{(0,0)\}}_{\{(1,0)\}\{(1,0)\}} - J^H_{\{(0,0)\}\{(0,0)\}}_{\{(3,0)\}\{(3,0)\}} \tag{18}$$

$$u_2 = (E_1 - \mu)P_{\{(0,0)\}\{(0,0)\}}_{\{(2,0)\}\{(2,0)\}} + P^H_{\{(0,0)\}\{(0,0)\}}_{\{(2,0)\}\{(2,0)\}}/2$$
$$+ J^H_{\{(0,0)\}\{(0,0)\}}_{\{(2,0)\}\{(2,0)\}} \tag{19}$$

$$u_3 = (E_1 - \mu)R_{\{(0,0)\}\{(0,0)\}}_{\{(1,1)\}\{(1,1)\}} + R^H_{\{(0,0)\}\{(0,0)\}}_{\{(1,1)\}\{(1,1)\}} \tag{20}$$

$$u_4 = J^H_{\{(0,0)\}\{(0,0)\}}_{\{(3,0)\}\{(3,0)\}}/2 \tag{21}$$

$$s_1 = (E_2 - 2\mu)C_{\{(2,0)\}\{(0,0)\}}_{\{(1,0)\}\{(1,0)\}} - 2M_{\{(2,0)\}\{(0,0)\}}$$
$$+ C^H_{\{(2,0)\}\{(0,0)\}}_{\{(1,0)\}\{(1,0)\}} \tag{22}$$

$$s_2 = (E_2 - 2\mu)C_{\{(2,0)\}\{(0,0)\}}_{\{(3,0)\}\{(1,0)\}} + C^H_{\{(2,0)\}\{(0,0)\}}_{\{(3,0)\}\{(1,0)\}} \tag{23}$$

$$s_3 = (2E_1 - 2\mu - J/2)S_{\{{(0,0)\atop(1,1)}\}\{{(0,0)\atop(2,0)}\}} + S^H_{\{{(0,0)\atop(1,1)}\}\{{(0,0)\atop(2,0)}\}} \quad (24)$$

$$s_4 = M_{\{{(0,0)\atop(3,0)}\}\{{(0,0)\atop(1,0)}\}} + M_{\{{(0,0)\atop(1,0)}\}\{{(0,0)\atop(3,0)}\}}$$
$$-2M_{\{(2,0)\}\{(0,0)\}} \quad (25)$$

$$s_5 = 2M_{\{{(0,0)\atop(0,1)}\}\{{(0,0)\atop(1,0)}\}} - 2M_{\{{(0,0)\atop(3,0)}\}\{{(0,0)\atop(1,0)}\}}$$
$$-2M_{\{{(0,0)\atop(1,0)}\}\{{(0,0)\atop(3,0)}\}} + 2M_{\{(2,0)\}\{(0,0)\}} \quad (26)$$

$$s_6 = M_{\{{(2,0)\atop(-1,0)}\}\{{(0,0)\atop(1,0)}\}}/2 \quad (27)$$

$$s_7 = 2M_{\{{(1,1)\atop(0,1)}\}\{{(0,0)\atop(1,0)}\}} - M_{\{{(2,0)\atop(-1,0)}\}\{{(0,0)\atop(1,0)}\}}$$
$$-(J/2)C_{\{{(2,0)\atop(3,0)}\}\{{(0,0)\atop(1,0)}\}} \quad (28)$$

$$d_1 = P_{\{{(0,0)\atop(2,0)}\}\{{(0,0)\atop(2,0)}\}}/2 \quad (29)$$

$$d_2 = R_{\{{(0,0)\atop(1,1)}\}\{{(0,0)\atop(1,1)}\}}/2 \quad (30)$$

$$o_1 = C_{\{{(2,0)\atop(1,0)}\}\{{(0,0)\atop(1,0)}\}} \quad (31)$$

$$o_2 = P_{\{{(2,0)\atop(3,0)}\}\{{(0,0)\atop(1,0)}\}} \quad (32)$$

$$o_3 = S_{\{{(0,0)\atop(1,1)}\}\{{(0,0)\atop(2,0)}\}} \quad (33)$$

Parameters which are presented below correspond to different categories of process which involve string states.

$$P_{\{{(0,0)\atop(2,0)}\}\{{(0,0)\atop(2,0)}\}} = -[2\sum_{\mu=2,\nu=0}(z-1)^{\mu+\nu-2}\alpha_\mu^2\alpha_\nu^2$$
$$+\sum_{\mu=1,\nu=1}(z-1)^{\mu+\nu-2}\alpha_\mu^2\alpha_\nu^2] \quad (34)$$

$$C_{\{{(2,0)\atop(1,0)}\}\{{(0,0)\atop(1,0)}\}} = -\sum_{\mu=0,\nu=1}(z-1)^{\mu+\nu-1}\alpha_{\mu,\nu}\alpha_{\mu+1,\nu-1} \quad (35)$$

$$C_{\{{(2,0)\atop(3,0)}\}\{{(0,0)\atop(1,0)}\}} = \sum_{\mu=0,\nu=2}(z-1)^{\mu+\nu-2}\alpha_{\mu,\nu}\alpha_{\mu+2,\nu-2} \quad (36)$$

$$S_{\{{(0,0)\atop(1,1)}\}\{{(0,0)\atop(2,0)}\}} = -\sum_{\mu=2,\nu=0}(z-1)^{\mu+\nu-2}\alpha_\mu\alpha_\nu\alpha_{\mu-2}\alpha_{\nu+2} \quad (37)$$

$$R_{\{{(0,0)\atop(1,1)}\}\{{(0,0)\atop(1,1)}\}} = -\left[\alpha_1^2 + (z-2)\sum_{\mu=2}(z-1)^{\mu-2}\alpha_\mu^2\right]^2 \quad (38)$$

$$M_{\{(2,0)\}\{(0,0)\}} = (J/2)\sum_{\mu=2}(z-1)^{\mu-2}\alpha_\mu\alpha_{\mu-2} \quad (39)$$

$$M_{\{{(0,0)\atop(3,0)}\}\{{(0,0)\atop(1,0)}\}} = (J/2)\sum_{\mu=0,\nu=2}(z-1)^{\mu+\nu-2} \times$$
$$\alpha_{\mu,\nu}\alpha_\mu\alpha_{\nu-2} \quad (40)$$

$$M_{\{{(0,0)\atop(1,0)}\}\{{(0,0)\atop(3,0)}\}} = (J/2)\sum_{\mu=2,\nu=0}\left[\delta_{\mu,2}(z-1)^\nu\right.$$
$$\left.+(1-\delta_{\mu,2})(z-2)(z-1)^{\mu+\nu-3}\right]\alpha_\mu\alpha_\nu\alpha_{\mu-2,\nu} \quad (41)$$
$$(42)$$

$$M_{\{{(0,0)\atop(0,1)}\}\{{(0,0)\atop(1,0)}\}} = (J/2)\sum_{\mu=2,\nu=0}\left[\delta_{\mu,2} + (1-\delta_{\mu,2})\times\right.$$
$$(z-2)(z-1)^{\mu-3}]\left[\delta_{\nu,0} + (1-\delta_{\nu,0})(z-2)(z-1)^{\nu-1}\right] \times$$
$$\alpha_{\mu,\nu}\alpha_{\mu-2,\nu} \quad (43)$$
$$(44)$$

$$M_{\{{(2,0)\atop(-1,0)}\}\{{(0,0)\atop(1,0)}\}} = (-J/2)\sum_{\mu=1,\nu=1}(z-1)^{\mu+\nu-2}\alpha_{\mu,\nu} \times \quad (45)$$
$$\alpha_{\mu-1}\alpha_{\nu-1} \quad (46)$$

$$M_{\{{(1,1)\atop(0,1)}\}\{{(0,0)\atop(1,0)}\}} = (-J/2)\sum_{\mu=1,\nu=1}\left[\delta_{\mu,1} + (1-\delta_{\mu,1})\times\right.$$
$$(z-2)(z-1)^{\mu-2}]\left[\delta_{\nu,1} + (1-\delta_{\nu,1})(z-2)(z-1)^{\nu-2}\right] \times$$
$$\alpha_{\mu,\nu}\alpha_{\mu-1,\nu-1} \quad (47)$$

$$C^H_{\{{(2,0)\atop(1,0)}\}\{{(0,0)\atop(1,0)}\}} = -t\sum_{\mu=1}(z-1)^{\mu-1}\alpha_{0,\mu}\alpha_{0,\mu-1} \quad (48)$$

$$C^H_{\{{(2,0)\atop(3,0)}\}\{{(0,0)\atop(1,0)}\}} = t\sum_{\mu=2}(z-1)^{\mu-2}\alpha_{0,\mu}\alpha_{1,\mu-2} \quad (49)$$

$$P^H_{\{{(0,0)\atop(2,0)}\}\{{(0,0)\atop(2,0)}\}} = -2t(\alpha_0^2\alpha_1\alpha_2 + \alpha_0\alpha_1^3) \quad (50)$$

$$S^H_{\{{(0,0)\atop(1,1)}\}\{{(0,0)\atop(2,0)}\}} = -t\sum_{\mu=2}\alpha_\mu\alpha_0\alpha_{\mu-2}\alpha_1 \quad (51)$$

$$R^H_{\{{(0,0)\atop(1,1)}\}\{{(0,0)\atop(1,1)}\}} = -t\sum_{\mu=1}\alpha_1\alpha_\mu^2\alpha_0 \quad (52)$$

$$J^H_{\{{(0,0)\atop(1,0)}\}\{{(0,0)\atop(1,0)}\}} = (-J/2)\Big[2\sum_{\mu=2,\nu=0}(z-1)^{\mu+\nu-2}\alpha_{\mu,\nu}^2 + \quad (53)$$
$$\sum_{\mu=1,\nu=1}(z-1)^{\mu+\nu-2}\alpha_{\mu,\nu}^2\Big] \quad (54)$$

$$J^H_{\{{(0,0)\atop(3,0)}\}\{{(0,0)\atop(3,0)}\}} = (-J/2)\Big[2\sum_{\mu=2,\nu=0}(z-1)^{\mu+\nu-2} \times \quad (55)$$
$$(\alpha_\mu\alpha_\nu)^2 + \sum_{\mu=1,\nu=1}(z-1)^{\mu+\nu-2}(\alpha_\mu\alpha_\nu)^2\Big] \quad (56)$$

$$J^H_{\{{(0,0)\atop(2,0)}\}\{{(0,0)\atop(2,0)}\}} = (-J/2)\sum_{\mu=1,\nu=0}\left[\delta_{\mu,1} +\right.$$
$$(1-\delta_{\mu,1})(z-2)(z-1)^{\mu-2}]\left[\delta_{\nu,0} +\right.$$
$$(1-\delta_{\nu,0})(z-2)(z-1)^{\nu-1}](\alpha_\mu\alpha_\nu)^2. \quad (57)$$

Spin polarons are defined as a solution of the following eigenvalue problem

$$zt\alpha_1 + 2J\alpha_0 = E_1\alpha_0,$$
$$t\alpha_{\mu-1} + (z-1)t\alpha_{\mu+1} + J\left(\frac{5}{2} + \mu\right)\alpha_\mu =$$
$$E_1\alpha_\mu, \quad (58)$$

where $\mu \geq 1$. A solution to the following Schrödinger equation for two particles in the same potential well determines the the wave function of the spin bipolaron,

$$t\left[\alpha_{\mu-1,\nu} + (z-1)\alpha_{\mu+1,\nu} + \alpha_{\mu,\nu-1} + (z-1)\alpha_{\mu,\nu+1}\right] +$$
$$J\left(4 + \mu + \nu - \frac{1}{2}\delta_{\mu+\nu,0}\right)\alpha_{\mu,\nu} = E_2\alpha_{\mu,\nu}, \quad (59)$$

where $\alpha_{\mu,\nu} = 0$ for $\mu < 0$ or $\nu < 0$. The normalization conditions for spin-polaron wave functions are

$$\alpha_0^2 + z\sum_{\mu=1}(z-1)^{(\mu-1)}\alpha_\mu^2 = 1 \quad (60)$$

$$\sum_{\mu=0,\nu=0}(z-1)^{(\mu+\nu)}\alpha_{\mu,\nu}^2 = 1. \quad (61)$$

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The thermodynamic potential of the model at $T = 0$ in the approximation applied in the paper is given by

$$\frac{\Omega_s - \Omega_n}{N}\Big|_{T=0} = \frac{1}{N}\sum_{\mathbf{k}} \frac{|\xi_{\mathbf{k}}| - \epsilon_{\mathbf{k}}}{2} -$$

$$\{\Delta_{1,0}^2(4u_1 + 8u_4 - 4s_1 + 4s_2 - 16s_4 - 8s_5 + 16s_6 + 8s_7)$$
$$+\Delta_{2,1}^2 24u_4 + \Delta_{3,0}^2 4u_4 + \Delta_{1,0}\Delta_{2,1}(16s_4 + 16s_6) +$$
$$\Delta_{1,0}\Delta_{3,0}(8s_4 + 8s_6)\}, \tag{62}$$

where $\xi_{\mathbf{k}}$ and $\epsilon_{\mathbf{k}}$ are quasiparticle energies in the normal and superconducting state

$$\xi_{\mathbf{k}} = E_1 + h(S_{\mathbf{k}}^{(2,0)} + 2S_{\mathbf{k}}^{(2,0)}) - \mu, \tag{63}$$
$$E_{\mathbf{k}} = \sqrt{\xi_{\mathbf{k}}^2 + \Delta_{\mathbf{k}}^2}.$$

The gap function is strongly anisotropic,

$$\Delta_{\mathbf{k}} = d_{\mathbf{k}}^{(1,0)}\Delta_{\mathbf{e}_x} + d_{\mathbf{k}}^{(2,1)}\Delta_{2\mathbf{e}_x+\mathbf{e}_y} + d_{\mathbf{k}}^{(3,0)}\Delta_{3\mathbf{e}_x} \tag{64}$$

$$d_{\mathbf{k}}^{(1,0)} = (2u_1 + 4u_4 - 2s_1 + 2s_2 - 8s_4 - 4s_5 +$$
$$8s_6 + 4s_7)D_{\mathbf{k}}^{(1,0)} + (2s_4 + 2s_6)D_{\mathbf{k}}^{(2,1)} +$$
$$(2s_4 + 2s_6)D_{\mathbf{k}}^{(3,0)} \tag{65}$$
$$d_{\mathbf{k}}^{(2,1)} = (4s_4 + 4s_6)D_{\mathbf{k}}^{(1,0)} + 6u_4 D_{\mathbf{k}}^{(2,1)} \tag{66}$$
$$d_{\mathbf{k}}^{(3,0)} = (2s_4 + 2s_6)D_{\mathbf{k}}^{(1,0)} + 2u_4 D_{\mathbf{k}}^{(3,0)}, \tag{67}$$

where

$$D_{\mathbf{k}}^{(1,0)} = 2\cos(k_x) - 2\cos(k_y) \tag{68}$$
$$D_{\mathbf{k}}^{(2,1)} = 2\cos(2k_x + k_y) + 2\cos(2k_x - k_y) -$$
$$2\cos(k_x + 2k_y) - 2\cos(k_x - 2k_y) \tag{69}$$
$$D_{\mathbf{k}}^{(3,0)} = 2\cos(3k_x) - 2\cos(3k_y) \tag{70}$$
$$S_{\mathbf{k}}^{(2,0)} = 2\cos(2k_x) + 2\cos(2k_y) \tag{71}$$
$$S_{\mathbf{k}}^{(1,1)} = 2\cos(k_x + k_y) + 2\cos(k_x - k_y). \tag{72}$$

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